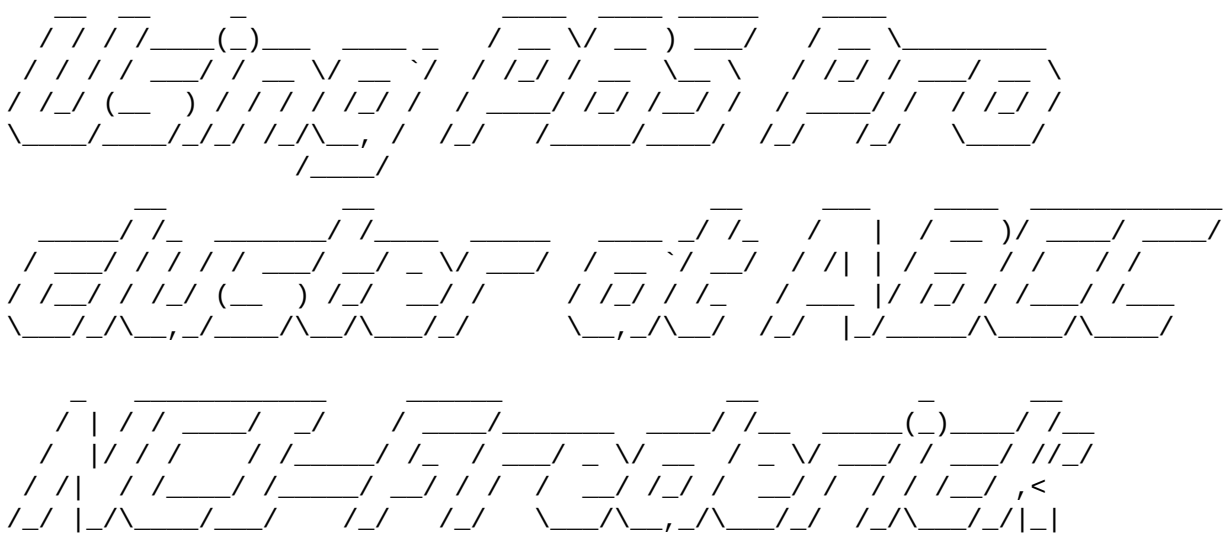

by Karol Miaskiewicz (SAIC/NCI-Frederick)

This document provides an introduction to the usage of the PBS Pro cluster on the server ncisgi.ncifcrf.gov, located within Advanced Biomedical Computing Center at NCI-Frederick. Keep in mind, that our PBS Pro cluster is an evolving configuration. As a result, this document may be a subject to frequent modifications and rewritings. Please, check it frequently for up-to-date information.

Karol Miaskiewicz

latest update Friday, June 4, 15:15, 2004

PDF version of this manual is available on ncisgi.ncifcrf.gov at /etc/abcc/pbs-intro.pdf

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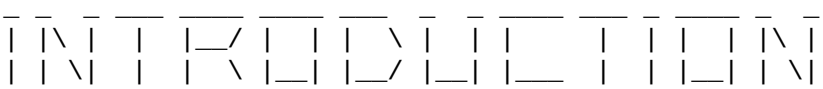


PBS Pro is a workload and resource management system in use on computational servers at the ABCC. The PBS server that runs on the host ncisgi.ncifcrf.gov sends batch tasks for execution on the following computational servers:

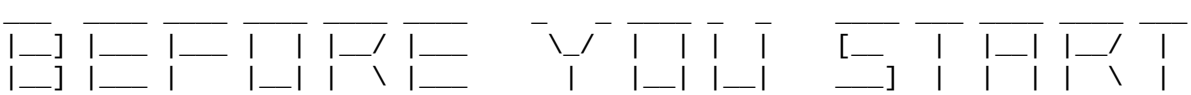
```
 nucleic1 - SGI Origin 300 with 8 x 500 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          280 GB of scratch disk space
 nucleic2 - SGI Origin 300 with 8 x 500 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          280 GB of scratch disk space
 nucleic3 - SGI Origin 300 with 8 x 500 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          140 GB of scratch disk space
 nucleic4 - SGI Origin 300 with 8 x 500 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          140 GB of scratch disk space
* nucleic5 - SGI Origin 300 with 8 x 500 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          140 GB of scratch disk space
 proteic1 - SGI Origin 300 with 8 x 600 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          280 GB of scratch disk space
 proteic2 - SGI Origin 300 with 8 x 600 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          280 GB of scratch disk space
 proteic3 - SGI Origin 300 with 8 x 600 MHz MIPS R14000 processors
          (4 MB of secondary cache per processor), 8 GB of memory,
          280 GB of scratch disk space
 avanti   - SGI Origin 3800 with 64 x 600 MHz MIPS R14000 processors
          (8 MB of secondary cache per processor), 64 GB of memory,
          1 TB of scratch disk space
 nciaxp   - DEC AlphaServer 8400 with 8 x 625MHz Alpha EV56 processors,
          (8 MB of secondary cache per processor), 12 GB of memory
 ncies45  - HP ES45 with 4 x 1250MHz Alpha EV68 processors,
          (16 MB of secondary cache per processor), 32 GB of memory
 ncip690  - IBM P690 with 16 x 1300MHz Power4 processors (HPC option
          i.e. with 1.4 MB of L2 cache per cpu, 32 MB of L3 cache),
          32 GB of memory, 1 TB of scratch disk space
 ncip691  - IBM P690 with 32 x 1300MHz Power4 processors (1.4 MB of
          L2 cache shared by 2 cpus, 32 MB of L3 cache), 64 GB of memory,
          1 TB of scratch disk space
 ncip692  - IBM P690 with 28 x 1300MHz Power4 processors (1.4 MB of
          L2 cache shared by 2 cpus, 32 MB of L3 cache)), 48 GB of memory,
          1 TB of scratch disk space
 dexter   - SGI Altix with 64 x 1500MHz Itanium2 processors, 64 GB of
          memory, 0.3 TB of scratch disk space
```

* Only 5 processors on node nucleic5 are dedicated for PBS batch use

All computing systems also have access to nine terabytes of shared disk space on two SGI TP9400 disk arrays. This space is shared as a CXFS clustered filesystem on SGI nodes, and as an NFS filesystem on non-SGI nodes.

The primary PBS commands are: 'qsub' to submit a job, 'qstat' to see the queues or job status, and 'qdel' to delete a job. Your path is set to include PBS commands. Man pages for PBS commands are also available.

In addition, Altair provides a User Guide for PBS Pro. This guide is
located at:
  /usr/local/pbs/doc/PBSproUserGuide.pdf
You are encouraged to read this document.



  ** IMPORTANT NOTE **
In order to use PBS on ncisgi, each user's .rhosts file needs to modified,
and possibly the .cshrc file. When you are ready to start using PBS, run
the script 'prepare_for_pbs'. This script will:
- make necessary modifications in your .rhosts file
- create /usr/tmp/[yourusername] directories on all computing nodes
- warn you if your .cshrc (or .profile) file needs to be modified

It is mandatory that the number of processors needed for your job be
specified with the '-l ncpus=#' PBS flag (see the next section). Double check
that the specified number of processors is what your job really uses. Jobs
without accurate ncpus definition will be terminated due to the wasted
resources.

Specify the memory limit for your job with '-l pvmem=' or '-l pmem=', which
are limits per process. If you run Gaussian, never use global memory limits
such as mem and vmem. Gaussian is a series of consecutive processes (Gaussian
links), mem and vmem limits are cummulative limits, i.e. PBS sums up memory
used in each process within the job. The end result is that your Gaussian job
is very likely to run out of mem or vmem, if they are specified.

Limit your jobs to no more than 8 processors. If you want to run on more
processors, seek approval by contacting Bob Lebherz (lebherz@ncifcrf.gov)
or Karol Miaskiewicz (miaskiew@ncifcrf.gov). Remember, that if you request
more than 8 processors you must force your job to run on the SGI Origin 3800,
IBM P690 nodes, or SGI Altix since these are the only systems with more than
8 processors available. Please, read the section "Running on a specific node
or specific architecture" near the end of this document.

Note, that there are nodes of different computer architectures available in
our cluster (currently SGI Irix, HP/Compaq Tru64, IBM Aix, and Linux on SGI
Altix). By default, all submitted jobs are scheduled to run on SGI Irix nodes.
To run your job on a different computer architecture, read the section
"Running on a specific node or specific architecture" near the end of this
document.

  ** IMPORTANT NOTE **
Not all applications are available on all computer architectures represented
in the cluster. For example, Gaussian98 is installed on the SGI and IBM nodes
but not the Alpha nodes (i.e. nciaxp and ncies45). On the other hand, GCG
is available exclusively on the Alpha nodes. Information about availability
of scientific programs on different platform can be accessed from our website
www.abcc.ncifcrf.gov (go to the "Scientific Applications" section). If the
information that you are looking for is not present, please, contact our staff
(http://support.abcc.ncifcrf.gov or 301-8465555).

Your home directory is shared among all compute nodes (and ncisgi, too).
There are disk quotas enforced on the /users filesystem (this is where the
home directories are located), check your quota with the 'quota -v' command.
/users is shared via CXFS mechanism on all SGI nodes which allows a very

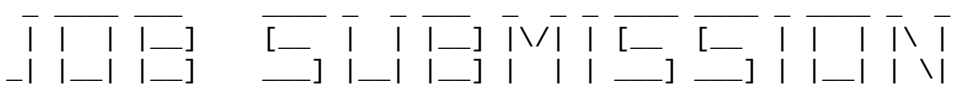
fast-performing filesystem (as if locally attached storage). However, non-SGI nodes use the much less efficient NFS mechanism to share /users.

Keep in mind, that NFS can cause performance degradation during very intensive I/O operations especially when accessing very large files. What it all means for you, is that your job can write output files directly to your home directory if this does not involve very intensive I/O operations (and if they fit into your available disk quota). This is especially true on CXFS nodes (i.e. SGI systems). However, if intensive I/O operations are involved you should write to a local filesystem, and specifically /usr/tmp, on the node where the job is executing. To illustrate this issue with a real-world example, it may be okay to write the Gaussian98 output file in your home directory, but all Gaussian scratch files should be written to the local /usr/tmp filesystem. In another example, it is ok to write outputs from molecular dynamics runs (such as done with programs CHARMM, AMBER, or Discover) directly into your home directory if you do not not save coordinates and velocities very frequently. However, it is likely that these files will be too large for your disk quota, and for this reason you should consider using the local scratch disk area (i.e. /usr/tmp).

There is another reason that you may want to avoid using NFS filesystems in your PBS jobs. NFS filesystems are very sensitive to any network related problems. If your job tries to write to an NFS mounted filesystem, it may abort when there are intermittent network problems (such as network congestion)

and access to an NFS server times out. For this reason, limiting your job to using just local filesystems (such as /usr/tmp) results in increased reliability.

The /usr/tmp filesystem is a dedicated scratch area on each of computing nodes. Keep in mind, that each node has its own /usr/tmp filesystem. As a case in point, if you place files in /usr/tmp/[yourusername] on ncisgi, these files will not be available in /usr/tmp/[yourusername] on other nodes, unless you specifically transfer them there. The /usr/tmp filesystem is configured for the best performace. We use disk striping across many disks and controllers, and large block size to provide optimal performance. /usr/tmp is the largest filesystem available to you on computing nodes - on many of our nodes it is one terabyte in size. Therefore, if you need performance and/or a lot of disk space, your job should be using the /usr/tmp filesystem, and specifically the /usr/tmp/[yoursusername] directory. Keep in mind, that, as a scratch area, /usr/tmp is not backed up. Also, files not accessed for over 30 days are automatically removed. Never store any of your important files under /usr/tmp.



Job submission is performed via the 'qsub' command:
  qsub <batch submission script>

A batch submission script contains the usual commands required to run the application that you are using. It also contains PBS job submission options in the header of the script. These options are placed in the lines that start with the #PBS string. These lines MUST be the first lines of the script.

For example, the following script will perform a Gaussian98 calculation (let's name it g98.job):

```
#PBS -S /bin/csh
#PBS -N h2o_mp2
#PBS -l cput=10:00:00
#PBS -l pvmem=400mb
#PBS -l ncpus=4
#PBS -m e

setenv g98root /usr/local/fbscapp/g98_A11.3
source $g98root/g98/bsd/g98.login
setenv GAUSS_SCRDIR /usr/tmp/miaskiew

cd /users/primgr/miaskiew/Water
g98 < h2o_mp2_opt.in > h2o_mp2_opt.out
```

It can be submitted to PBS with the simple command 'qsub g98.job'. All of the necessary options are provided at the begining of the script (lines starting with #PBS):

```
#PBS -S /bin/csh
```
The -S flag denotes the shell to be used

```
#PBS -N h2o_mp2
```
The -N flag denotes the name with which the job will appear in the batch system (this does not have to be the name of the script, it can be practically any name you deem relevant, but it cannot start with a digit). The name will be truncated to ten characters in the qstat output, if it is longer.

```
#PBS -l cput=10:00:00
```
The -l flag indicates the limits of resources required for the job. cput is the CPU time required for the job. It can be provided as an integer of number of seconds or in the notation hours:minutes:seconds (or minutes:seconds)

```
#PBS -l pvmem=400mb
```
Pvmem sets the limit of virtual memory per process. In this case it is 400 megabytes. It should be specified as an integer followed by one of the suffixes: b, kb, mb, gb, w, kw, mw, gw (for bytes, kilobytes, megabytes, gigabytes, words, kilowords, megawords, and gigawords, respectively)

```
#PBS -l ncpus=4
```
Number of cpus required

```
#PBS -m e
```
The -m flag asks to send an email message to the user. Followed by the 'e' argument means to send the message when the job is completed.

Note, that it is not necessary to list PBS flags separately in each line. They can be grouped, such as in the following:

```
#PBS -S /bin/csh -N h2o_mp2
#PBS -l cput=10:00:00,pvmem=400mb,ncpus=4
#PBS -m e
```

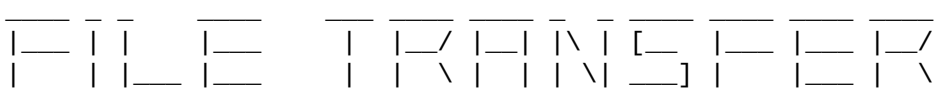
Note also, that it is not required and not recommended to submit a job to a specific queue. PBS will make the decision about queue placement based on your requested resources.

There are more PBS flags that can be used in the script. Man pages on qsub

provide information on available flags/options. At minimum, the following flags must be used in the PBS script to run on our SGI and IBM nodes:

```
  -S         (to specify a shell for the job)
  -l cput=   (to specify the per job time limit)
  -l pvmem=  (to specify the virtual memory per process)
  -l ncpus=  (to specify the number of CPUs)
```

More flags are required to run on Alpha nodes (i.e. nodes nciaxp and ncies45). Contact us for additional details regarding the Alphas.



The example discussed so far does not take into account file delivery issues. If all your input and output files reside within your user home directory (see the discussion in the section "Before you start") or one of other globally shared filesystems such as /abcc, you do not need to be concerned with file transfer issues. However, if your job will use local (i.e. non-shared) filesystems you must take care of delivery of files to and from an execution host.

Using our example of a Gaussian job, if the only output file that we are interested in is the Gaussian log file (i.e. h2o_mp2_opt.out) there is no need to transfer any files, since the log file is written in your globally shared home directory filesystem. However, let's assume that we want to restart the calculation from a Gaussian checkpoint file. Since the checkpoint file is intensively accessed by Gaussian during execution we want to use the local /usr/tmp filesystem for optimal performance. Also, we want the checkpoint file to be saved and returned after the execution of our job.

There are a few approaches that can be applied to file delivery in our configuration. To illustrate them with our Gaussian job example:

-- 1 -- Since your home directory is shared between all potential execution hosts, you could simple used the Unix cp command to copy the checkpoint file from your home directory to /usr/tmp/[yourusername] on the execution host:

```
#PBS -S /bin/csh
#PBS -N h2o_mp2
#PBS -l cput=10:00:00
#PBS -l pvmem=400mb
#PBS -l ncpus=4
#PBS -m e

setenv g98root /usr/local/fbscapp/g98_A11.3
source $g98root/g98/bsd/g98.login
setenv GAUSS_SCRDIR /usr/tmp/miaskiew

cd /users/primgr/miaskiew/Water
cp h2o_mp2_opt.chk /usr/tmp/miaskiew
g98 < h2o_mp2_opt.in > h2o_mp2_opt.out
cp /usr/tmp/miaskiew/h2o_mp2_opt.chk .
```

(Note, that all commands in the script are executed on an execution host and not on ncisgi where the job is submitted. This is why the cp command above does transfer files to and from /usr/tmp/miaskiew on an execution host.)

-- 2 -- The same can be achieved with the Unix rcp command. Note, that if you need to transfer the checkpoint file to and from a non-shared filesystem on ncisgi, the rcp command is the one that you must use (you could also use stagein/stageout directives as described below).

In our example, let us assume that we want keep the checkpoint file on the /usr/tmp/miaskiew filesystem on ncisgi. As explained before, this is a different /usr/tmp filesystem than that found on an execution host.

```
#PBS -S /bin/csh
#PBS -N h2o_mp2
#PBS -l cput=10:00:00
#PBS -l pvmem=400mb
#PBS -l ncpus=4
#PBS -m e

setenv g98root /usr/local/fbscapp/g98_A11.3
source $g98root/g98/bsd/g98.login
setenv GAUSS_SCRDIR /usr/tmp/miaskiew

rcp ncisgi:/usr/tmp/miaskiew/h2o_mp2_opt.chk /usr/tmp/miaskiew
cd /users/primgr/miaskiew/Water
g98 < h2o_mp2_opt.in > h2o_mp2_opt.out
rcp /usr/tmp/miaskiew/h2o_mp2_opt.chk ncisgi:/usr/tmp/miaskiew
```

-- 3 -- The most universal and foolproof way to transfer files is with PBS Pro stagein and stageout directives.

```
#PBS -S /bin/csh
#PBS -N h2o_mp2
#PBS -l cput=10:00:00
#PBS -l pvmem=400mb
#PBS -l ncpus=4
#PBS -m e
#PBS -W stagein=/usr/tmp/miaskiew/h2o_mp2_opt.chk@ncisgi:/usr/tmp/miaskiew/h2o_m
p2_opt.chk
#PBS -W stageout=/usr/tmp/miaskiew/h2o_mp2_opt.chk@ncisgi:/usr/tmp/miaskiew/h2o_
mp2_opt.chk

cd /users/primgr/miaskiew/Water
g98 < h2o_mp2_opt.in > h2o_mp2_opt.out
```

(Note the order of hosts in the stagein directive! It appears to be awkward, but this is how it works. The first hostname is always an execution host. In the case of stagein directive it means that the first host listed in the stagein specification is the host where the files are transferred to, and not the host where the files are transferred from.)

As an additional example other than Gaussian, let's consider an AMBER job which we want to run from the /usr/tmp/miaskiew directory. We need to deliver all AMBER input files to /usr/tmp/miaskiew on an execution host, and then return the output files to the home directory.

```
-- 1 --  Using the cp command:

#PBS -S /bin/csh -N dna12mer
#PBS -l cput=100:00:00,pvmem=400mb,ncpus=4
#PBS -m e

setenv AMBERHOME /usr/local/fbscapp/amber6
set path = ($path $AMBERHOME/exe)

cd /usr/tmp/miaskiew

cp /users/primgr/miaskiew/dna12mer/dna_eq.in .
cp /users/primgr/miaskiew/dna12mer/dna_eq.top .
cp /users/primgr/miaskiew/dna12mer/dna_eq.crd .

mpirun -np 4 sander -O -i dna_eq.in -o dna_eq.out \
   -p dna_seq.top -c dna_eq.crd -x dna_eq.traj -r dna_eq.rst

cp dna_eq.rst /users/primgr/miaskiew/dna12mer
cp dna_eq.traj /users/primgr/miaskiew/dna12mer
cp dna_eq.out /users/primgr/miaskiew/dna12mer


-- 2 -- With the rcp command:

#PBS -S /bin/csh -N dna12mer
#PBS -l cput=100:00:00,pvmem=400mb,ncpus=4
#PBS -m e

setenv AMBERHOME /usr/local/fbscapp/amber6
set path = ($path $AMBERHOME/exe)

cd /usr/tmp/miaskiew

rcp ncisgi:dna12mer/dna_eq.in dna_eq.in
rcp ncisgi:dna12mer/dna_eq.top dna_eq.top
rcp ncisgi:dna12mer/dna_eq.crd dna_eq.crd

mpirun -np 4 sander -O -i dna_eq.in -o dna_eq.out \
   -p dna_seq.top -c dna_eq.crd -x dna_eq.traj -r dna_eq.rst

rcp dna_eq.rst ncisgi:dna12mer/dna_seq.rst
rcp dna_eq.traj ncisgi:dna12mer/dna_seq.traj
rcp dna_eq.out ncisgi:dna12mer/dna_seq.out


-- 3 -- With the PBS stagein and PBS stageout directives:

#PBS -S /bin/csh -N dna12mer
#PBS -l cput=100:00:00,pvmem=400mb,ncpus=4
#PBS -m e
#PBS -W stagein=/usr/tmp/miaskiew/dna_eq.in@ncisgi:dna12mer/dna_eq.in
#PBS -W stagein=/usr/tmp/miaskiew/dna_eq.top@ncisgi:dna12mer/dna_eq.top
#PBS -W stagein=/usr/tmp/miaskiew/dna_eq.crd@ncisgi:dna12mer/dna_eq.crd
#PBS -W stageout=/usr/tmp/miaskiew/dna_eq.rst@ncisgi:dna12mer/dna_eq.rst
#PBS -W stageout=/usr/tmp/miaskiew/dna_eq.traj@ncisgi:dna12mer/dna_eq.traj
#PBS -W stageout=/usr/tmp/miaskiew/dna_eq.out@ncisgi:dna12mer/dna_eq.out

cd /usr/tmp/miaskiew
```

```
setenv AMBERHOME /usr/local/fbscapp/amber6
set path = ($path $AMBERHOME/exe)

mpirun -np 4 sander -O -i dna_eq.in -o dna_eq.out \
   -p dna_seq.top -c dna_eq.crd -x dna_eq.traj -r dna_eq.rst


** IMPORTANT NOTE **
All of the above examples will work fine when delivering input files from
a submission host (ncisgi) to an execution host. However, they may fail when
returning output files to ncisgi if the CPU time limit (as defined
with the -l cput=100:00:00) is exhausted.

In our AMBER example, if the job terminates prematurely due to the CPU time
limit while in execution of the sander program, no commands in the script
after the 'mpirun -np 4 sander' line will be executed, and thus no output
files will be ruterned the to home directory when cp and rcp commands are
used.  To avoid this problem:

  - use PBS stageout directives - they are always executed, even when
    the CPU time limit is exhausted

  - use cp or rcp, but define different CPU time limits for job (cput) and
    for process (pcput) with the job limit being at least 20 seconds longer.
    In our AMBER example, we would need to add the pcput limit to the
    PBS limits definitions:
    #PBS -l cput=100:01:00,pvmem=400mb,ncpus=4,pcput=100:00:00
    If the limit per job is longer than the limit per process, even when
    the sander process reaches the process CPU time limit, there is still
    CPU time available per job to execute the consecutive commands.



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Currently, the longest cpu time allowed is 999 hours (3596400 seconds). The
largest pvmem value allowed is 10000 megabytes, and one can use no more than
8 processors. These limits may change. To verify current limits, use the
'qstat -q' command to list all of the queues, and then display limits in
each queue with the 'qstat -Qf queuename' command. If your job needs more
than the indicated available limits, we have a special queue called massive.
This queue is normally disabled. Contact Karol Miaskiewicz
(miaskiew@ncifcrf.gov) or Bob Lebherz (lebherz@ncifcrf.gov) to run in this
queue.



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```

While we normally discourage such use and rely on PBS load balancing, forced execution on a particular node or a particular computer architecture is justified when one is doing benchmarking or when an application is available only on a particular node or a particular architecture.

Running on a particular node can be achieved with the -l nodes=name, where the name is either 1) a hostname or 2) a node property of the node where you want to run your job. Thus, to force a job to run on the SGI Origin 3800 (hostname avanti) one would use the following option:

```
 #PBS -l nodes=avanti
```

or

```
 #PBS -l nodes=sgi-origin3800-600mhz
```

In this second example, the value sgi-origin3800-600mhz is a property of the node avanti.

You can get the hostnames of all the members of our PBS cluster and their respective properties and resources displayed with the 'pbsnodes -a' command. For example, the pbsnodes output for node nucleic5, indicates that it is an SGI Origin 300 system with 500 MHz processors (properties = sgi-origin300-500mhz) with eight GB of memory (resources_available.mem = 8388608kb), and eight processors (pcpus = 8):

```
nucleic5
     ntype = time-shared
     state = free
     license = l
     pcpus = 8
     properties = sgi-origin300-500mhz,gaussian
     resources_available.arch = irix6
     resources_available.mem = 8388608kb
     resources_available.ncpus = 6
     resources_available.pvmem = 6000mb
     resources_assigned.ncpus = 0
```

Using '-l nodes=property' may be advantageous when performing benchmarks. For example, We have two kinds of SGI Origin 300 nodes - some with 500MHz MIPS processors and the others with 600 MHz MIPS processors. To force an execution to take place on an SGI Origin 300 node with 600 MHz processors, one could use:

```
 #PBS -l nodes=sgi-origin300-600mhz
```

Note, also that we have marked nodes where the Gaussian98 and Gaussian03 programs are installed with the property tag 'gaussian'. Thus, if you simply want to execute your job on any compute server that has Gaussian program installed, the best and simplest approach is to use '-l nodes=gaussian'.

Often you may want to run on a particular computer architecture - for example when your application is unique to the Compaq/HP True64 platform. In this case, you do not care which node will execute your job, as long as it is a Compaq/HP True64 node. You can specify this with the architecture resource flag:

```
  #PBS -l arch=digitalunix
```

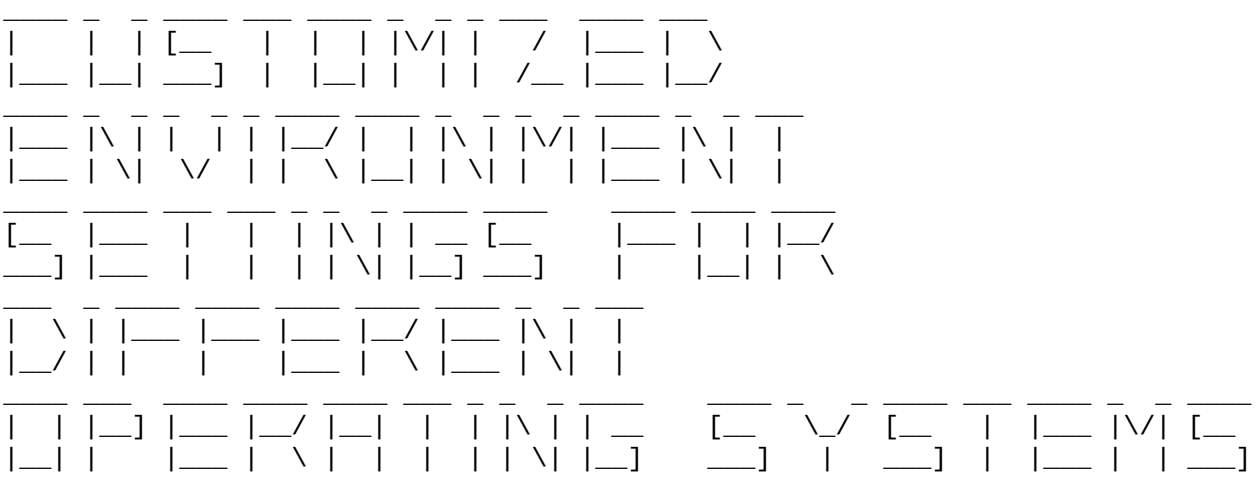
To see the available architecture resources, use the pbsnodes command. The output of pbsnodes will display it for each node in the form:

```
  resources_available.arch = irix6
```

or
  resources_available.arch = digitalunix
or
  resources_available.arch = aix4
or
  resources_available.arch = linux_cpuset

Currently, there are multiple nodes of four different architectures available in our cluster - irix6 (SGI Irix nodes) digitalunix (Alpha based DEC/HP Tru64 nodes), aix4 (IBM AIX nodes), and linux_cpuset (SGI Altix node).

Note, that irix6 is the default architecture. This means that all jobs are placed on SGI Irix nodes, unless otherwise specified with the architecture resource flag (arch=) or the nodes= flag.



Currently, there are nodes with three different operating systems present in our cluster - Irix, Tru64, and AIX. Note, that your home directory is shared among these three platforms. If you need to have your environmental settings to be unique for each platform:

1) Copy your current .cshrc, .profile, and .login to .cshrc.IRIX64, .profile.IRIX64, and .login.IRIX64, respectively. These files will contain your settings specific for SGI/Irix systems. Use them to customize your settings there.

2) copy the .cshrc, .profile, and .login from /usr/abcc/skel to your home directory. Do not edit them!

3) create .cshrc.OSF1, .profile.OSF1, .login.OSF1 for Alpha/Tru64 specific settings if you wish. They are not required, i.e. you should be able to run jobs on Tru64 nodes without them. Use them only if you need/want to customize your settings there.

4) create .cshrc.AIX, .profile.AIX, .login.AIX for IBM AIX specific settings. Again they are not required to execute jobs, however, use them if you need to customize settings on IBM nodes.

5) create .cshrc.Linux, .profile.Linux, .login.Linux for SGI Altix specific settings, if you need them.

6) If you want to have common aliases/settings for both platforms - place them in cshrc.common or profile.common files (depending on what shell you are using).

```
_  _ _ ____ _ _ _ _ _  _ ____    ___  ___  ____
|  | | |___ | | | | |\ | | __    |__] |__] [__
 \/  | |___ |_|_| | | \| |__]    |    |__] ___]
____ _  _ ____ _  _ ____ ____
|  | |  | |___ |  | |___ [__
|_\| |__| |___ |__| |___ ___]
```

The qstat command is used to see PBS queues. Useful options:

qstat -a	lists all of the jobs within the PBS cluster
qstat -an	lists all of the jobs within the PBS cluster and their respective execution hosts
qstat -q	lists all of the queues within the PBS cluster (including resource limits)
qstat -s	lists all of the jobs within the PBS with their respective status comments
qstat -Qf queue	lists all information about a specific queue
qstat -f jobid	lists detailed information about a specific job

Additional options are available. Please, read more about qstat in man pages (man qstat).

```
_ _  _ ___ ____ ____ ____ ____ ___ _ _  _ ____    ____ _  _ _  _ ____
| |\ |  |  |___ |__/ |__| |     |  | |  | |___    |__/ |  | |\ | [__
| | \|  |  |___ |  \ |  | |___  |  |  \/  |___    |  \ |__| | \| ___]
_  _ _  _ ___  ____ ____    ___  ___  ____
|  | |\ | |  \ |___ |__/    |__] |__] [__
|__| | \| |__/ |___ |  \    |    |__] ___]
```

PBS can also be used for interactive work. There are some applications that cannot be used in a batch environment. One can use such applications under PBS's resource management control with the interactive flag.

To illustrate the use of interactive PBS jobs with an example: Suppose that one needs to run a very long MATLAB computation that requires that it be started from MATLAB's graphical interface. Also, we want to run on an SGI Irix system. This can be achieved with the following simple command:

```
 qsub -N myjob -I -l cput=20:00:00,pvmem=2000mb,ncpus=1,arch=irix6
```

As soon as the requested resources are available, you will be presented with a prompt on an SGI node and you can start your interactive MATLAB session. Keep in mind, that your session will be terminated with no warning when it exceeds the requested resources that you have specified.

In another example, one needs to compile and debug his program on an SGI Altix system. While this can be achieved via a PBS batch script, it may be easier and more convenient to do it interactively. In order to get an interactive shell on SGI Altix, one could try one of the following:

```
 qsub -N compile -I -l cput=20:00:00,pvmem=200mb,ncpus=1,arch=linux_cpuset
or
 qsub -N compile -I -l cput=20:00:00,pvmem=200mb,ncpus=1,nodes=dexter
```

or
```
 qsub -N compile -I -l cput=20:00:00,pvmem=200mb,ncpus=1,nodes=ALTIX
```

(This last command works because this node has a property ALTIX assigned to it, as indicated by the output of the 'pbsnodes dexter' command.)

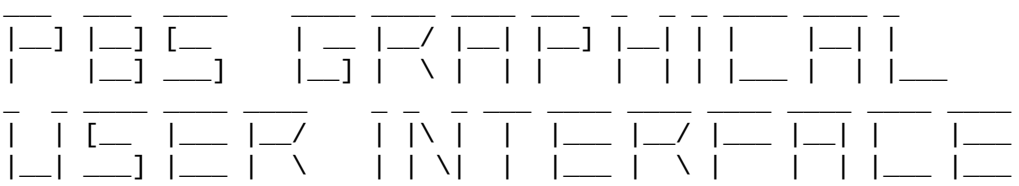
Occassionally, PBS may not be able to immediately intialize your interactive session. When this occurs, you would simply see the message:

```
   qsub: waiting for job 29001.ncisgi to start
```

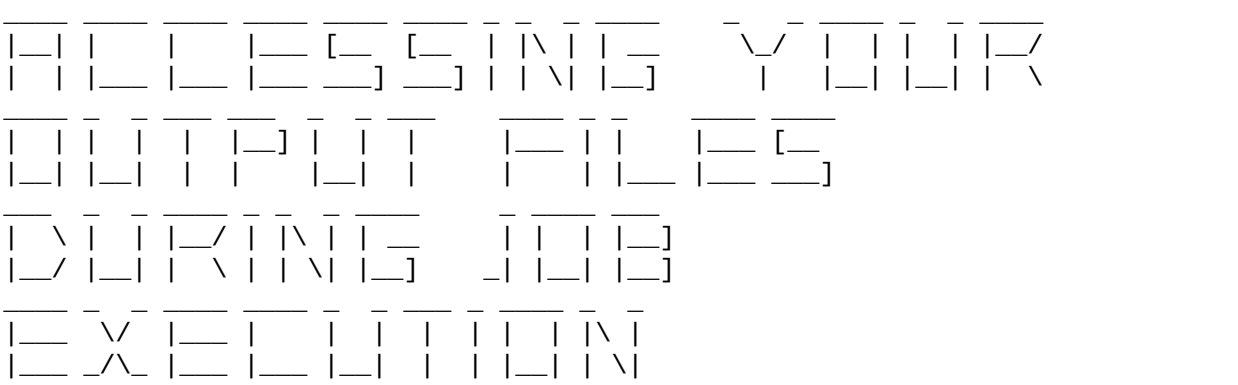
If the task that you want to execute via PBS interactive session is not CPU intensive (for instance, you just want to compile/debug your program), specifying ncpus=0 in your qsub request may allow your request to succeed immediately, such as in one of our examples:

```
 qsub -N compile -I -l cput=20:00:00,pvmem=200mb,ncpus=0,nodes=dexter
```

Keep in mind though, that this trick works often but not always; it depends on a specific reason that prevents PBS from initializing your interactive session. Usually it is because the system you want to connect to is actually too busy to support any more jobs of any kind, even non-cpu intensive jobs. No system will allow jobs in when it is too busy.



If you are interacting with an X11 enabled system (any Unix/Linux box, or a PC running X-server software), you are encouraged to use xpbs, a graphical user interface for pbs. xpbs allows one to view jobs in PBS queues, resources available in the queues, and other information about the PBS cluster. xpbs will also help you to submit a PBS job.



This is a very relevant question in our configuration when the execution host may be different than the one where you are logged in (i.e. ncisgi). If your job uses your home directory for output files, you will be able to see them on ncisgi as this is a shared filesystem. However, if your output files are on the /usr/tmp or another local filesystem on an execution host, you do not have direct access to these files while on ncisgi. To take a look at your output files, follow these steps:

- First, determine which host is executing your job. You can see this information using the 'qstat -an' command.

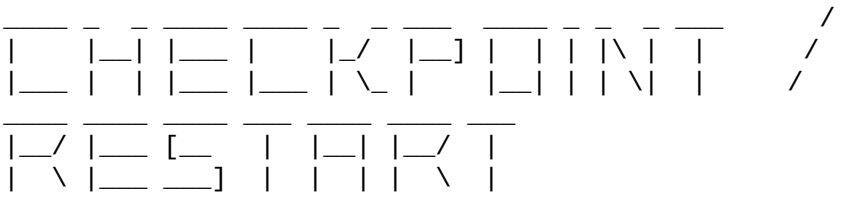
- Next, use the rcp command to copy the file back to ncisgi and view it. For example, if you find out that your job runs on the host named nucleic1, and the output that you would like to view is /usr/tmp/miaskiew/h2o_mp2.out:

```
   rcp nucleic1:/usr/tmp/miaskiew/h2o_mp2.out .
```

This command will transfer the file to your current directory. Then use 'vi' or 'more' or whatever viewer/editor you like.

- If it is enough to see just the end of the file to check progress of your calculations, the 'tail' command can provide that information:

```
  rsh nucleic1 tail -40 /usr/tmp/miaskiew/h2o_mp2.out
```



Some operating systems - currently Unicos and Irix - support process checkpoint and restart capability. Since the majority of our server are SGI servers running Irix, you should be able to make use of checkpoint/restart in your PBS jobs.

Checkpoint creates an image on a disk of a running process. When the process dies, it is possible to restart it from this checkpoint file. If, for some reason, our PBS cluster fails (hardware failure, power outage, etc.), the job can be restarted from the last checkpoint file, and, thus, does not need to be rerun from the begining saving user possibly a lot of CPU time.

Note, that some applications offer their own checkpoint capabilities. Gaussian offers checkpointing, many molecular dynamics programs also create restart files. A system checkpoint is totally different than an application checkpoint. With application checkpoint, such as in Gaussian, a user needs to restart his/her calculation which usually requires modifications (although often very minor) to a Gaussian input file. Also, some methods in Gaussian are not checkpointable via Gaussian checkpoint file.

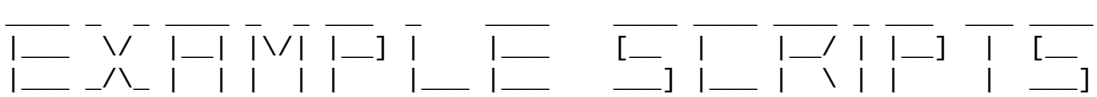
System checkpoint allows the job to restart transparently to a user. He/she does not need to adjust input files, and restart jobs. PBS will take care of all of it when it is restarted after a shutdown.

Unfortunately, not every application is checkpointable. Applications that keep open sockets (such as Discover, or Dgauss) are not checkpointable. However, some such as Gaussian, AMBER, CHARMM often are.

The PBS -c flag controls checkpoint behavior. If you absolutely do not want to have checkpoints performed on your job you should set it to n, i.e. '-c n'. If you want checkpoints performed at regular default intervals set on the PBS server, set it to c, i.e. '-c c', which we strongly recommend. Note, if you do not provide the -c flag, it defaults to '-c s' which means to perform a checkpoint only when PBS shuts down. The problem with this behavior is that if the system crashes due to a hardware failure, PBS is not shutdown gracefully, and a checkpoint does not execute. This is why we suggest that you use the '-c c' flag.

Currently, our queues are set to perform a checkpoint after every 240 minutes
of CPU time.

  ** IMPORTANT NOTE **
Note, that non-checkpointable jobs are restarted from the very beginning
after PBS restarts on an execution host. Also, if a restart from the system
checkpoint fails for any reason, the job is restarted from the very beginning.
This usually means that your output files generated so far will be
overwritten and you will loose all results from the interrupted run. If you
want to avoid such situations, mark your job as non-rerunnable and
non-checkpointable with '-r n -c n' options.



```
==============
| Gaussian98 |
==============
```

```
 ---
 SGI
 ---
```

```
#PBS -S /bin/csh -N mp2
#PBS -l cput=220:01:00,pcput=220:00:00,pvmem=4000mb,ncpus=8

cd /users/primgr/miaskiew/Work

setenv g98root /usr/local/fbscapp/g98_A11.3
source $g98root/g98/bsd/g98.login
setenv GAUSS_SCRDIR /usr/tmp/miaskiew

g98 < c3endo_mp2.in > c3endo_mp2.out

cp /usr/tmp/miaskiew/c3endo.chk .
```

```
 ---
 IBM
 ---
```

The same script as above will run Gaussian98 job on IBM servers. You just
need to add arch=aix4 to the #PBS line to force execution on IBMs, i.e.:

```
#PBS -l cput=220:01:00,pcput=220:00:00,pvmem=4000mb,ncpus=8,arch=aix4
```

```
==============
| Gaussian03 |
==============
```

```
 ----------
 SGI Origin
 ----------
```

```
#PBS -S /bin/csh -N mp2
#PBS -l cput=220:01:00,pcput=220:00:00,pvmem=4000mb,ncpus=8
```

```
cd /users/primgr/miaskiew/Work

setenv g03root /usr/local/fbscapp/g03_B04
source $g03root/g03/bsd/g03.login
setenv GAUSS_SCRDIR /usr/tmp/miaskiew

g03 < c3endo_mp2.in > c3endo_mp2.out

cp /usr/tmp/miaskiew/c3endo.chk .
```

IBM

The same script as above will run Gaussian03 job on IBM servers. You just need to add arch=aix4 to the #PBS line to force execution on IBMs, i.e.:

```
#PBS -l cput=220:01:00,pcput=220:00:00,pvmem=4000mb,ncpus=8,arch=aix4
```

SGI Altix

The same basic Gaussian03 script should also work on the SGI Altix server. What is needed is to specify arch=linux_cpuset:

```
#PBS -l cput=220:01:00,pcput=220:00:00,pvmem=4000mb,ncpus=8,arch=linux_cpuset
```

==========
| AMBER7 |
==========

SGI Origin

```
#PBS -S /bin/csh -N amb_bench
#PBS -l cput=80:00:00,ncpus=4,pvmem=600mb

cd /users/primgr/miaskiew/AMBER

set SANDER = "/usr/local/fbscapp/amber7/exe/sander"

mpirun -np 4 $SANDER -O \
            -i 16s80na_eqe.in \
            -o 16s80na_eqe.out \
            -p 16s80nab.top \
            -c 16s80na_eqd.rst \
            -r 16s80na_eqe.rst \
            -x 16s80na_eqe.traj \
            -inf 16s80na_eqe.inf
```

(Note, that the number of processors is controlled via the -np flag to mpirun. Make sure that this number and and the number of processors requested from PBS via ncpus= are the same.)

SGI Altix

AMBER PBS script for SGI Altix is similar the one above for SGI Origin.
One needs to change architecture requested to arch=linux_cpuset. In addition,
some MPI environment variables need to be setup to control the memory usage.

```
#PBS -S /bin/csh -N amb_bench
#PBS -l cput=80:00:00,ncpus=4,pvmem=600mb,arch=linux_cpuset

cd /users/primgr/miaskiew/AMBER
set SANDER = "/usr/local/fbscapp/amber7/exe/sander"

setenv MPI_MAPPED_HEAP_SIZE 67108864
setenv MALLOC_MMAP_MAX 0
setenv MALLOC_TRIM_THRESHOLD -1
setenv  MPI_MEMMAP_OFF 1

mpirun -np 4 $SANDER -O \
            -i 16s80na_eqe.in \
            -o 16s80na_eqe.out \
            -p 16s80nab.top \
            -c 16s80na_eqd.rst \
            -r 16s80na_eqe.rst \
            -x 16s80na_eqe.traj \
            -inf 16s80na_eqe.inf
```

IBM

```
#PBS -S /bin/csh -N amb_ibm
#PBS -l cput=80:00:00,ncpus=4,pvmem=600mb,arch=aix4

cd /users/primgr/miaskiew/AMBER

set SANDER = "/usr/local/fbscapp/amber7/exe/sander"

setenv MP_PROCS 4
setenv MP_SHARED_MEMORY yes
setenv MP_WAIT_MODE poll

$SANDER -O -i 16s80na_eqe.in \
           -o 16s80na_eqe.out \
           -p 16s80nab.top \
           -c 16s80na_eqd.rst \
           -r 16s80na_eqe.rst \
           -x 16s80na_eqe.traj \
           -inf 16s80na_eqe.inf
```

(Note, that the number of processors is controlled via the MP_PROCS variable.
Make sure that this number and and the number of processors requested from
PBS via ncpus= are the same.)

==========
| CHARMM |
==========

(Keep in mind, that our center does not have a license to share a copy of CHARMM with outside users. You must have your own CHARMM license, and your own copy of the program which must be installed under your own user area. If you have problems compiling and installing CHARMM, our personnel may help you with these tasks. Scripts below are just examples of using CHARMM - modify them with location of your own copy of CHARMM.)

```
 ----------
 SGI Origin
 ----------

#PBS -S /bin/csh -N charmm_sgi
#PBS -l cput=02:02:00,pvmem=1000mb,ncpus=8

setenv CHARMM /usr/local/fbscapp/harvard/c27b3/exec/sgi64/charmm

cd /users/primgr/miaskiew/CHARMM

mpirun -np 8 $CHARMM < mbcodyn.inp > mbcodyn.out
```

(Note, that the number of processors is controlled via the -np flag to mpirun. Make sure that this number and and the number of processors requested from PBS via ncpus= are the same.)

```
 ---
 IBM
 ---

#PBS -S /bin/csh -N charmm_ibm
#PBS -l cput=20:00:00,pvmem=1200mb,ncpus=8,arch=aix4

setenv CHARMM /usr/local/fbscapp/harvard/c27b3/exec/ibmsp/charmm

cd /users/primgr/miaskiew/CHARMM

setenv MP_PROCS 8
setenv MP_SHARED_MEMORY yes
setenv MP_WAIT_MODE poll

$CHARMM < mbcodyn.inp > mbcodyn.out
```

(Note, that the number of processors is controlled via the MP_PROCS variable. Make sure that this number and the number of processors requested from PBS via ncpus= are the same.)

GAMESS

```
 ----------
 SGI Origin
 ----------

#PBS -S /bin/csh -N myjob
#PBS -l ncpus=4,pvmem=500mb,cput=50:00:30,pcput=50:00:00

set GAMESS=/usr/local/fbscapp/gamess/rungms
cd /users/primgr/miaskiew/Gamess
```

```
$GAMESS uracil_rohf_ccpVDZ_opt 4 uracil_rohf_ccpVDZ_opt.out
```

(Note, that the number of processors is controlled via the second argument
to our rungms script. Make sure that this number and the number of processors
requested from PBS via ncpus= are the same.)

SGI Altix

The above GAMESS PBS script for SGI Origin will also work on our SGI Altix
system. The only change needed is to request arch=linux_cpuset, i.e.:

```
#PBS -l ncpus=4,pvmem=500mb,cput=50:00:30,pcput=50:00:00,arch=linux_cpuset
```

IBM

The same script as above will run GAMESS job on IBM servers. You just
need to add arch=aix4 to force execution on IBMs, i.e.:

```
#PBS -l ncpus=4,pvmem=500mb,cput=50:00:30,pcput=50:00:00,arch=aix4
```

========
| NAMD |
========

SGI Origin

```
#PBS -S /bin/csh -N namd -l pvmem=600mb,cput=2:00:00,ncpus=4

set path = ($path /usr/local/fbscapp/namd_2.5/bin)
cd /users/primgr/miaskiew/NAMD/er-gre
namd2 +p4 er-gre.namd
```

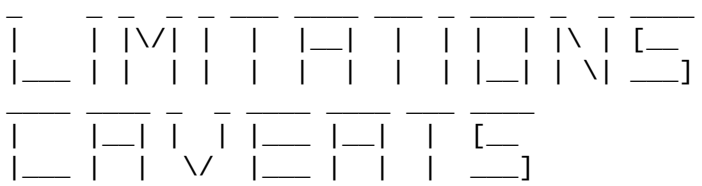
(Note, that the number of processors is controlled with the +p flag, such
as 4 processors in the above example with +p4.)

IBM

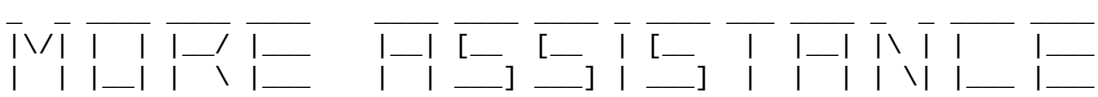
```
#PBS -S /bin/csh -N namd -l pvmem=600mb,cput=2:00:00,ncpus=4,arch=aix4

set path = ($path /usr/local/fbscapp/namd_2.5/bin)
cd /users/primgr/miaskiew/NAMD/er-gre
poe namd2 er-gre.namd -nodes 1 -procs 4 -shared_memory yes
```

(NAMD is executed on IBM systems via IBM's POE - Parallel Operating
Environment. The number of processors is controlled with POE's -procs
flag, such as '-procs 4' in the above example.)



If you specify a non-existant file in a stagein directive the job may not fail but rather remain on the PBS server in "W" (i.e. Waiting) state. PBS will attempt every few minutes to try transfer the file again. If you create the missing file, your job may start. If it does not, you should delete it with qdel and resubmit after fixing the problem.



If you require more assistance, contact our technical personnel preferably on the web at http://support.abcc.ncircrf.gov or by phone at 301-846-5555. SGI specific questions may also be sent directly to Karol Miaskiewicz (miaskiew@ncifcrf.gov). IBM questions should be addressed to Dennis Foley (foleyd@ncifcrf.gov), while SGI/Altix and HP/Alpha questions to Toni Harbaugh (harbaugh@ncifcrf.gov).